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13. ABSTRACT (Maximum 200 words) <p>The year of 1992-1993 is a highly-productive year for the project of the Computer Simulation Study of High Temperature Superconductor Structure. In this year, the main barrier to the simulation was overcome. A pair-interaction potential between a pair of charges such as electron-electron, hole-hole, and electron-ion, etc. in a layered two-dimensional system was obtained. It amazingly presents negative values within a certain interparticle distances that should have been absolutely positive according to the Coulomb's law. Of most importance is that while discovering this, the essence of high temperature superconductivity was probably touched. It was shown that quite a lot of anomalous behaviors of high temperature superconductors can be explained and understood by means of this interaction potential. The mysterious phase transition from an insulator to a superconductor is well understood and the transition temperature is calculated showing consistency with measurements.</p>			
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## I. A List of Objectives

The year of 1992-1993 is a highly-productive year for this project. During this year, the following work has been done:

1) A pair-interaction potential between a pair of charges such as electron-electron, hole-hole, and electron-ion, etc. in a layered two-dimensional system was obtained.

2) Therefore, the main barrier to the simulation was overcome.

3) The obtained potential amazingly presents negative values within a certain interparticle distances that should have been absolutely positive according to the Coulomb's law.

4) Of most importance is that while discovering this, the essence of high temperature superconductivity was probably touched. It was shown that quite a lot of anomalous behaviors of high temperature superconductors can be explained and understood by means of this interaction potential. The mysterious phase transition from an insulator to a superconductor is well understood and the transition temperature is calculated showing consistency with measurements.

## II. Technical Accomplishments

The accomplishments during the past year consist of the following aspects;

### 1) Discovery of microscopic two-body (pair) interaction potential in a layered two-dimensional (2D) system

As many other scientists did in the simulation study of this subject, the phenomenological study was first tried in acquisition of interaction potential, but it was not successful. Therefore, the effort was turned to theoretical search from the microscopic point of view. It succeeded. The pair interaction potential between two electrons (holes), Fig. 1, shows an amazing negative part within a certain range of interparticle distances which implies that two electrons could attract each other to form a stable bond state. If one is familiar with the Bardeen-Cooper-Schrieffer (BCS) theory, he/she should immediately be alert that this potential presents a great promise to open the mystery of high temperature superconductivity.

Indeed, by using this marvelous potential, the following important issues in high  $T_c$  superconductivity have been solved in a few months:

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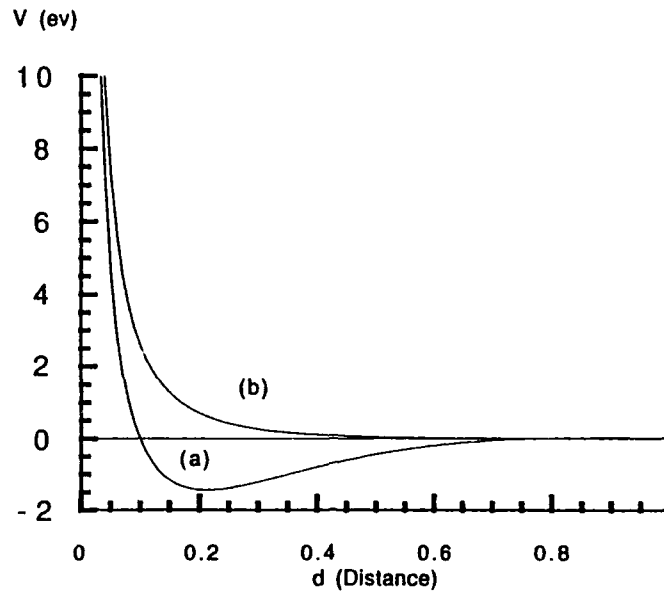


Fig. 1. Pair interaction potential between two particles with the same charges in a layered 2D system with electron correlations for  $c=6.6 \text{ \AA}$ ,  $m_b=2m_e$ ,  $n_s = 1.0 \times 10^{14} \text{ cm}^{-2}$ ; (a) in-plane potential; (b) potential in the direction normal to planes.

**a) explanation of whole mysterious phase transition diagram from an insulator to a normal metal with a high temperature superconducting region with the change of doping density in cuprates.**

The whole phase transition diagram has been reproduced in terms of the theory developed in this project, Fig. 2. The BCS result is just a natural outcome under a certain condition of the doping density  $x$ . However, the BCS theory has never given a result of varying  $T_c$  with doping density, but this theory does. Especially, the estimation of the critical point,  $x=0.053$ , at which  $\text{La}_{2-x}\text{St}_x\text{CuO}_4$  cuprates become superconductors directly from an insulator is in excellent agreement with experimental measurements.

**b) understanding and explanation of the phase transition from an insulator to a normal metal without a superconducting state at all or only with a low temperature superconducting state for some materials with the layered structure.**

Since the foundation of this success is the pair potential with the negative values, which was obtained by using the layered 2D structure and electron correlation effects, it is a logical question why some kind of layered 2D structure materials do not present high temperature superconductivity. This is also well and consistently explained in the developed theory.

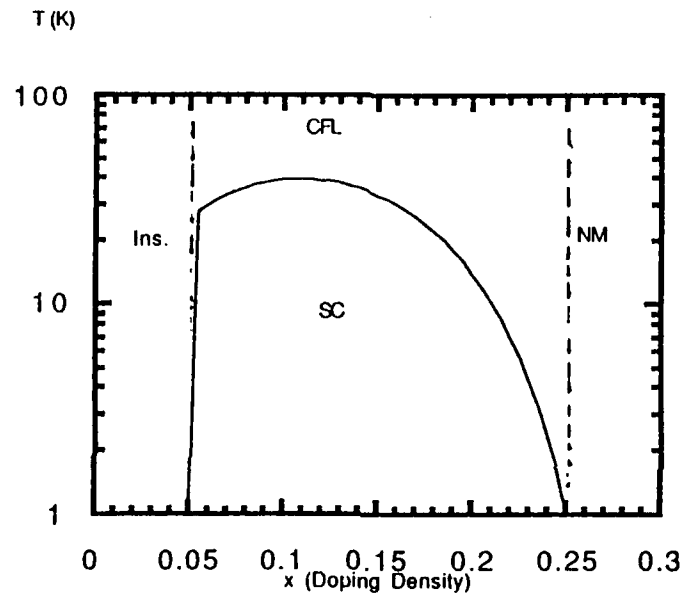


Fig. 2 Transition temperature  $T_c$  vs. the doping density  $x$  for LaSrCuO with  $c = 6.6$  Å, etc. to fit to the maximum  $T_c = 39$  K.

NM -Normal Metal, SC-Superconductivity, CFL-Correlated Fermi Liquid & Ins.-Insulator

### c) explanation of the increase of transition temperature with the increase of ambient pressure

It is also obtained from the theory that transition temperature should increase as ambient pressure (interlayer spacing) increases (decreases). It is also predicted that there is a minimum interlayer spacing at which superconductivity exists. This has not been experimentally observed because it is not easy to technically make such a cuprate with so short spacing. A saturation of transition temperature is obtained as well when spacing is getting large.

**d) understanding of the insulating state at a low doping density**

From the theory, when the doping density is low, it can reach a critical value at which the so-called charge-density-wave instability occurs that leads to localization of electrons due to the infinitely large effective mass of electron. Thus, the system reaches its boson dielectric state and the material becomes an insulator.

**2) Quasi-linear dependence of resistivity of cuprates with temperature in the normal state;**

**a) quasilinear dependence of in-plane resistivity with temperature**

This is explained by considering the electron-phonon interaction in the anisotropic structure - layered 2D sheets of materials. The phonon spectrum shows a band above the acoustic mode. From damping of a quasiparticle resistivity can be calculated and presents the dependence of  $T^3$  at low temperature and quasi-linearity at intermediate  $T$ , and linearity at high  $T$ .

**b) quasilinear dependence and high values of resistivity in the direction normal to planes**

Taking into account the tunneling of electrons in the direction normal to planes and using the potential in this direction, Fig. 1 (b), the high values and quasi-linearity of resistivity can be explained and well understood.

**3) Plasmon model of high temperature superconductivity**

Considering plasmon mediated electron in cuprates, a transition temperature  $T_c$  was also derived, which is similar to the BCS result and can explain a part of experimental results as BCS does. This is a part of efforts before the amazing potential is obtained. It can not compared with the recent outcomes, but it is a theoretical effort as a model.

**4) relation of transition temperature to the number of sublayers in multiple-layered structured cuprates**

The analytical relation between transition temperature and the number of sublayers per unit cell in multi-layered cuprates was derived and it

is found that it works very well in understanding of the temperature increase with the increase of the number of sublayers. However, written manuscripts have not been completed yet.

### III. Status of the Research

The research project is on the right track so far and the desired objectives are partially completed. Since most tough part of research has been accomplished, the remaining is relatively easy. It is expected that this project will be accomplished in the next year without any great difficulties. However, on account of the additional fruitiness, it might be necessary to take a few months more to complete the simulational studies without any additional funding, while furnishing more theoretical results in the field of high temperature superconductivity.

### IV. List of Written Publications

- 1) J. D. Fan, Z. H. Cai, G. Reiter and S. C. Moss, "Computer Simulation Studies of the Melting Transition of Rb and K Intercalated in Graphite" Phys. Rev. B, 48 (1993)
- 2) J. D. Fan, Z. H. Cai, "Constant Temperature Molecular Dynamics Simulation of the 2D Melting Transition of Rb and K," Proc. of 1992 Fall Meeting, MRS. May, 1993
- 3) Y. Malozovskiy, J. D. Fan, "Electron-Phonon Interaction and Quasiparticle Damping in a Layered Two-Dimensional Metal," Phys. Rev. Lett. (submitted)
- 4) Y. Malozovskiy, J. D. Fan, "Pair Interaction Potential in a Layered Two-Dimensional Metal," Phys. Rev. - Rapid Communications (submitted)
- 5) Y. Malozovskiy, J. D. Fan, "Superconductivity and Phase Transition in a Layered Two-Dimensional Correlated Liquid," Phys. Rev. Lett. (submitted)
- 6) Y. Malozovskiy, S. M. Bose, P. Longe and J. D. Fan, "Superconductivity in a Layered Two-Dimensional Metal," Phys. Rev. B (submitted)

- 7) Y. Malozovskiy, J. D. Fan, "Mechanism of High Temperature Superconductivity and Phase Transition in a Layered Two-Dimensional Cuprates" Proc. of Molecular & Oxides Superconductivity, Eugene, OR, Jul. 27 - Aug. 1, 1993. (submitted)
- 8) Y. Malozovskiy, J. D. Fan, "Insulator-Metal Phase Transition in a Layered Two-Dimensional System," Phys. Rev. (submitted)

## V. Professional Personnel

Principal Investigator, J. D. Fan, Ph. D., Assistant Professor, Department of Physics, Southern University

Research Associate, Y. M. Malozovskiy, Ph. D., Department of Physics, Southern University

Research Associate, Part time (40% of one half of year), D. S. Guo, Ph. D., Department of Physics, Southern University

## VI. Interactions

### A. Presentations

#### 1. National

- 1) J. D. Fan and Y. Malozovskiy, "Phonon Exchange Superconductivity in a Multilayered Two-Dimensional Metal," 1993 March Meeting of APS, Seattle, WA, Mar. 22 - 26, 1993
- 2) J. D. Fan and Y. Malozovskiy, "Electron-Phonon Interaction and Phonon Spectra in a Layered Two-Dimensional Metal," 1993 March Meeting of APS, Seattle, WA, Mar. 22 - 26, 1993
- 3) Y. Malozovskiy and J. D. Fan, "Phase Transition in the System of Intergrain Josephson Junction," 1993 March Meeting of APS, Seattle, WA, Mar. 22 - 26, 1993
- 4) Y. Malozovskiy and J. D. Fan, "Boson Exchange Superconductivity in a layered Two-Dimensional Metal," 1993 March Meeting of APS, Seattle, WA, Mar. 22 - 26, 1993

- 5) J. D. Fan and Y. Malozovskiy "Interionic Potential in a Layered Two-Dimensional Metal," US Air Force STAG Meeting, Dayton, Ohio, Mar. 16-18, 1993
- 6) J. D. Fan and Z. X. Cai, "Constant Temperature Simulation of a Two-Dimensional Melting of Rb and K," 1992 Fall MRS Meeting, Boston, MA, Nov. 30 -Dec. 4, 1992

## 2. Regional

- 1) D. S. Guo and J. D. Fan, "Energy Shift in Hydrogen Atom in a Strong Radiation Field," Fall meeting of APS TX Section, Nov. 7-8, 1992, Houston, TX
- 2) D. S. Guo, J. D. Fan, J. Linser and R. Ford, " Earth Spin and Ozone Depletion," Feb. 1993, 67-th Annual Meeting of Louisiana Academy of Science, Lafayette, Louisiana.

## 3. Local

- 1) J. D. Fan, "A novel Means of Information Transmission in Fiber-optical Communications Systems," Big Muddy Quantum Feast, Feb. 13, 1993, LSU
- 2) Y. Malozovskiy and J. D. Fan, "Electron-Phonon Interaction in a Layered Two-Dimensional Metal", Big Muddy Quantum Feast, Feb. 13, 1993, LSU

## 4. On-campus

- 1) G. S. Guo and J. D. Fan,, "Earth Spin and Ozone Depletion in Stratosphere", Apr. 1993, Department of Physics, Southern University.
- 2) J. D. Fan, "A novel Means of Information Transmission in Fiber-optical Communications Systems," Feb. 1993, Department of Physics, Southern University
- 3) J. D. Fan, "A novel Means of Information Transmission in Fiber-optical Communications Systems," Mar. 1993, Department of Electrical Engineering, Southern University
- 4) J. D. Fan, "A novel Means of Information Transmission in Fiber-optical Communications Systems," Apr. 1993, Timbuktu Academy, Department of Physics, Southern University



- 5) Y. Malozovski and J. D. Fan, "Introduction to High Temperature Superconductivity," Sep. 1992, Department of Physics, Southern University.
- 6) G. S. Guo and J. D. Fan "Non-Perturbative Theory of Quantum Electrodynamics," Sep. 1992, Department of Physics, Southern University.
- 7) Z. X. Cai, Brookhaven National Laboratory, invited talk, J. D. Fan (host), "High Temperature Superconductivity and Monte carlo Simulations" June, 1992, Department of Physics, Southern University.

### **B. Consultative and Advisory Functions**

- 1) Conference of Steering Committee of Science and Engineering Alliance, Feb. 7, 1993, Jackson State University, Jackson, MI

## **VII. Discoveries, Inventions and Patents**

The theoretical finding in high temperature superconductivity made in the past year is an essential contribution to this field. Although it needs further assessment from authorities, it is first time that one can fully explain and understand the high temperature superconductivity phase transition in terms of the theory developed in the present project. Its influence is profound and grand. The foundation of discovery is the pair interaction potential in a layered two-dimensional system.

## **VIII. Additional Statements**

After all, this project has achieved a great success in the exploration of high temperature superconductivity. Ambiguity and confusion for many years have in part been clarified. To date the upcoming results continuously support the achievements obtained. The mysterious issues are being solved one by one, but it takes time to do so because of the limited manpower available in this project. The final acceptance of the theory by the condensed matter society may need a couple of years or longer, however, it will be eventually acknowledged, I believe, that the developed theory is correct and successful and its value may not be under the BCS theory.